Alternating spin chains with singlet ground states

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We investigate low-energy properties of the alternating spin chain model composed of spin s_1 and s_2 with a singlet ground state. After examining the spin-wave spectrum in detail, we map low-energy spin excitations to the O(3) nonlinear sigma model in order to take into account quantum fluctuations. Analyzing the topological term in the resulting sigma model, we discuss how the massless or massive excitations are developed, especially according to the topological nature of the alternating spin system.

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I. INTRODUCTION

One-dimensional quantum spin systems show various interesting phenomena, having been continually providing hot topics. The most important example is the spin one-half antiferromagnetic Heisenberg chain, which was exactly solved by the Bethe-ansatz method. It is now well known that this model shows critical behavior specified by the level-1 Wess-Zumino-Witten model. Keeping the integrability by adding multiple terms, higher-spin models were constructed [1] and their critical behavior was also classified. Progress in a slightly different direction was made by Haldane [2–5], who conjectured that general higher-spin models behave in quite distinct ways according to whether the spin of the models is integer or half-odd integer. The massive phase of integer spin models, so-called the Haldane phase, has been indeed observed by experiments, and now is understood as the valence-bond-solid state [6]. The problem whether a given quantum spin system is massless or massive provides nontrivial and interesting issues, which have been stimulating the study of quantum phase transitions.

More recently, the mixed spin chains with an alternating array of two kind of spins have attracted much current interest [7,8]. The systems experimentally found so far [7] show a magnetically ordered ground state even for the antiferromagnetic case. For such ordered systems, quantum fluctuations may not play a crucial role. However, it is quite interesting to address the question what happens when the magnetic order disappears due to frustrations, etc. If such systems are realized experimentally, quantum fluctuations should certainly play an important role, exhibiting interesting phenomena such as the competition between the massless and massive phases. These systems may thus provide a new interesting paradigm of quantum spin chains. In this connection, an exactly solvable alternating spin chain, which has a singlet ground state, has been studied in detail [9].

The alternating spin models can also be regarded as a high concentration limit of magnetic impurities in spin chains. In this respect, the problem of the alternating spin models is closely related to that for the spin chains with impurities, which have been extensively studied for e.g. the two-leg ladder system [10–12], the spin-Peierls system [13,14], etc. In fact by changing the concentration of periodic array of impurities, we can naturally interpolate the alternating spin systems and spin systems with dilute impurities, and discuss their characteristic properties in a unified way [15].

In this paper, we study low-energy properties of the mixed spin chain models with an alternating array of two kind of spins. We deal with two kind of alternating spin models with a singlet ground state. By introducing quantum fluctuations to the spin-wave excitations, we investigate low-energy properties of the system by resorting to O(3) non-linear sigma model techniques. We then discuss how the massless or massive excitations are developed in the alternating spin models by analyzing the topological term in the sigma model.

The paper is organized as follows. In Section II, two types of the models for alternating spin chains are introduced, and some rigorous statements are given for the excited states as well as the ground state. In Section III, we calculate the spin-wave dispersion relation, and in Section IV, by converting the model to the non-linear sigma model, we study the low-energy characteristics of the spin excitations. The last section is devoted to summary of the paper.

A brief report on preliminary results for this paper is given in [15], where the effects of massive modes were not taken into account in the nonlinear sigma model approach.

II. MODELS AND BASIC PROPERTIES

In this section, we first introduce two kind of alternating spin models with a singlet ground state, and then

study them by means of Lieb-Schultz-Mattis (LSM) theorem.

The models we study in this paper are the quantum spin models with nearest neighbor interaction in one dimension. The corresponding Hamiltonian is defined by

$$H = \sum_{j=1}^{N_a} J_j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}, \tag{2.1}$$

where N_a is the number of lattice sites, and the spin at the j-th site is denoted by s_j. We will investigate the following two types of alternating spin-chain models by setting

$$\begin{aligned}
&\underline{\text{Model A:}}\\
&s_j = \begin{cases} s_1 & \text{for } j = 1 \\ s_2 & \text{for } j = 2, 3 \end{cases} \pmod 3 ,\\
&J_j = J,\\
&N_a = 6N,
\end{aligned} \tag{2.2}$$

$$\begin{aligned}
&\underline{\text{Model B:}}\\
&s_j = \begin{cases} s_1 & \text{for } j = 1, 2 \\ s_2 & \text{for } j = 3, 4 \end{cases} \pmod 4 ,\\
&J_j = \begin{cases} J(1-\gamma_1) & \text{for } j = 1 \\ J[1+(\gamma_1+\gamma_2)/2] & \text{for } j = 2, 4 \\ J(1-\gamma_2) & \text{for } j = 3 \end{cases} \pmod 4,\\
&N_a = 4N.
\end{aligned} \tag{2.3}$$

In both cases, the spin chain is composed by two kind of spins s_1 and s_2, which can take either integer or half integer spin. Note that we also include the effect of the bond-alternation for the Model B, which was originally introduced by Tonegawa et al. [16] In what follows, we assume the antiferromagnetic couplings $J > 0$ and $0 < \gamma_1, \gamma_2 < 1$.

Let us start by specifying the ground state properties. Since spins are on a bipartite lattice, we can apply the Marshall theorem [17–19,15] to (2.1), that is, we prove that the ground state is singlet without degeneracy for both models. Next consider the properties of excitations above the ground state by applying the LSM theorem [20]. Note that the Hamiltonian is invariant under 3- (4-)site translation for the Model A (B). Therefore, together with the fact that the ground state is unique, we can construct an excited state of $O(1/N)$ when $s_{\rm uc}$ = odd-integer, where $s_{\rm uc}$ is the summation of the spins in the unit cell

$$s_{\rm uc} = \begin{cases} s_1 + 2s_2 & \text{for A} \\ 2(s_1 + s_2) & \text{for B} \end{cases} \tag{2.4}$$

According to the above formula, we can state [15] that the Model A can be gapless if s_1 is a half-integer. In other cases where s_1 is an integer for the Model A, or s_1 and s_2 are arbitrary for the Model B, we cannot claim anything by the LSM theorem, which suggests that such systems may be gapful, as is the case for the ordinary Haldane system.

III. SPIN-WAVE SPECTRUM

So far we have seen that the Model A can show different phases, according to whether s_1 is integer or half-integer. However, the LSM theorem itself cannot distinguish a gapless phase from a gapful phase with degenerate ground states. In order to clarify this point, we wish to use a complementary approach based on effective field theory. For this purpose, we first investigate the dispersion relation of the spin-wave spectrum for the model, which allows us to judge whether the system can be mapped to the non-linear sigma model. The next subsection is devoted to deriving the spin-wave Hamiltonians by the Holstein-Primakoff mapping, and they are diagonalized in the subsection B. We then show some examples of the spin-wave spectrum calculated numerically.

A. Spin-wave Hamiltonian

1. Model A

For the usual uniform spin chain ($s_1 = s_2$ case for the present model), it is sufficient to introduce the two kind of bosons, corresponding to bipartite lattices. However, for the model with $s_1 \neq s_2$ we have to introduce the six kind of bosons such that

$$\begin{aligned}
&S^z_{6j+m} = (-)^m \left[n^{(m)}_{6j+m} - s_m \right],\\
&S^+_{6j+m} = \begin{cases} \sqrt{2s_m - n^{(m)}_{6j+m}}\, a^{(m)}_{6j+m} & \text{for odd } m \\ a^{(m)\dagger}_{6j+m} \sqrt{2s_m - n^{(m)}_{6j+m}} & \text{for even } m \end{cases},
\end{aligned} \tag{3.1}$$

where $j = 0, 1, \cdots, N-1$, $m = 1, 2, \cdots, 6$, $s_m = s_1$ (s_2) for $m = 1, 4$ (otherwise) and $n^{(m)}_{6j+m} = a^{(m)\dagger}_{6j+m} a^{(m)}_{6j+m}$. In what follows, we approximate the boson Hamiltonian up to quadratic order in order to derive the dispersion relation of spin wave excitations. In this assumption, the resultant Hamiltonian can be diagonalized in the momentum space. For this purpose, let us introduce the Fourier-transformed operators

$$a^{(m)}_{6j+m} = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \exp\left[\frac{2\pi i}{N} \frac{k}{6} (6j+m) \right] a^{(m)}_k, \tag{3.2}$$

with N being defined in eq.(2.2). Substituting these equations, we find

$$\begin{aligned}
H_{\rm sw} = \sum_{k=0}^{N-1} \sum_{l,m=1}^{6} (&a^\dagger_l h_{lm} a_m + a_l h_{lm} a^\dagger_m \\
&+ a^\dagger_l \Delta_{lm} a^\dagger_m + a_l \bar{\Delta}_{lm} a_m),
\end{aligned} \tag{3.3}$$

where we have used a notation,

$$a_m = \begin{cases} a_k^{(m)} & \text{for odd } m \\ a_{-k}^{(m)} & \text{for even } m \end{cases} \tag{3.4}$$

for short, and 6×6 matrices h and Δ are given by

$$h = Js_2 \mathrm{diag}\left(1, \frac{1+\alpha}{2}, \frac{1+\alpha}{2}, 1, \frac{1+\alpha}{2}, \frac{1+\alpha}{2}\right),$$

$$\Delta = \frac{Js_2}{2} \begin{pmatrix} 0 & \sqrt{\alpha}\rho & & & & \sqrt{\alpha}\bar{\rho} \\ \sqrt{\alpha}\rho & 0 & \bar{\rho} & & & \\ & \bar{\rho} & 0 & \sqrt{\alpha}\rho & & \\ & & \sqrt{\alpha}\rho & 0 & \sqrt{\alpha}\bar{\rho} & \\ & & & \sqrt{\alpha}\bar{\rho} & 0 & \rho \\ \sqrt{\alpha}\bar{\rho} & & & & \rho & 0 \end{pmatrix}. \tag{3.5}$$

We have defined in these equations

$$\alpha = \frac{s_1}{s_2}, \quad \rho = e^{ip} \tag{3.6}$$

with $p = (2\pi/N_a)k$. Matrix elements not written explicitly in eq.(3.5) are all 0. Note that the operators (3.4) as well as the matrix Δ depend on the momentum, though we have not explicitly denoted it.

2. Model B

In a similar way to the Model A, we now write down the spin-wave Hamiltonian for the Model B. Introduce the Holstein-Primakoff mapping with the use of four kinds of bosons similar to eq.(3.1) by replacing $6 \to 4$. With the same Fourier-transformed operators as eq.(3.2), we have the spin-wave Hamiltonian similar to eq.(3.3) for which h and Δ are 4×4 matrices defined by

$$h = \frac{Js_2}{2} \mathrm{diag}\left(\alpha\Gamma_1 + \Gamma, \alpha\Gamma_1 + \Gamma, \alpha\Gamma + \Gamma_2, \alpha\Gamma + \Gamma_2\right),$$

$$\Delta = \frac{Js_2}{2} \begin{pmatrix} 0 & \alpha\Gamma_1\rho & 0 & \sqrt{\alpha}\Gamma\bar{\rho} \\ \alpha\Gamma_1\rho & 0 & \sqrt{\alpha}\Gamma\bar{\rho} & 0 \\ 0 & \sqrt{\alpha}\Gamma\bar{\rho} & 0 & \Gamma_2\rho \\ \sqrt{\alpha}\Gamma\bar{\rho} & 0 & \Gamma_2\rho & 0 \end{pmatrix}, \tag{3.7}$$

where $\Gamma_i = 1 - \gamma_i$ and $\Gamma = 1 + (\gamma_1 + \gamma_2)/2$.

B. Diagonalization

In the previous subsection, we have derived the spin-wave Hamiltonians up to the quadratic order in boson operators. We can diagonalize these Hamiltonians by the Bogoliubov transformation.

Before discussing the spectrum of the present models, let us recall the alternating spin-chains with ferrimagnetic ground state [8], i.e, the same model given by (2.1), but with

$$s_{2j-1} = s_1, \quad s_{2j} = s_2, \quad J_j = J. \tag{3.8}$$

The spin-wave dispersion relation for this model is

$$\omega_\pm = \pm|s_1 - s_2| + \left[(s_1 - s_2)^2 + 4s_1 s_2 \sin^2 p\right]^{1/2}. \tag{3.9}$$

Thus the excitation spectrum is given by a quadratic function for small momentum. It is only the case for $s_1 = s_2$ that it has a linear dispersion.

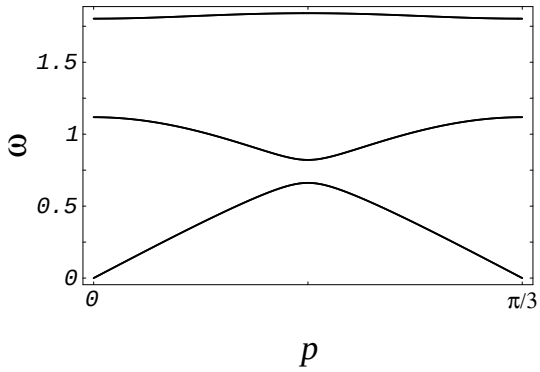

FIG. 1. Spin-wave spectrum of the Model A in unit J as functions of the momentum p for $s_1 = 1/2$ and $s_2 = 1$.

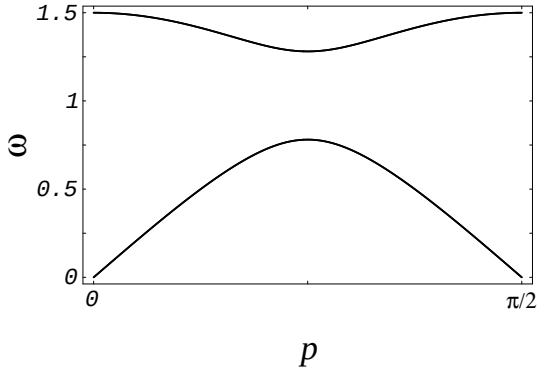

FIG. 2. Spin-wave spectrum of the Model B in unit J as functions of the momentum p for $s_1 = 1/2$ and $s_2 = 1$. Bond-alternation parameters are $\gamma_1 = \gamma_2 = 0$.

Now turn to the present model. We show the spectrum obtained numerically in Figs.1 and 2. We can see that the dispersion relation $\omega_0 \propto \sin p$ defined in $p \in [0, \pi]$ for the uniform chain is folded 3 (2) times for the Model A (B), and interactions among such modes produce gaps at the crossing point. Though we here presented only the case with $s_1 = 1/2$ and $s_2 = 1$, the qualitative features are the same for other cases $s_1 \neq s_2$. Contrary to this, in the case $s_1 = s_2$, interactions between the different modes disappear and the single dispersion ω_0 appears. What is remarkable is that the lowest mode has a linear dispersion, in contrast to the ferrimagnetic case, without an excitation gap. This property persists even if we include the bond-alternation, as can be seen in Figs.3 and 4. However, it goes without saying that because we have such a spin-wave spectrum, we cannot conclude a

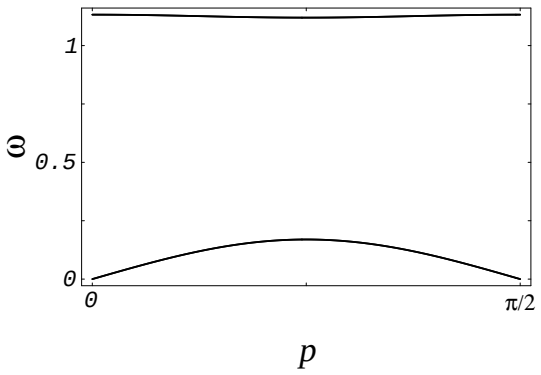

FIG. 3. The same figure as Fig.2, but with $\gamma_1 = \gamma_2 = 0.9$.

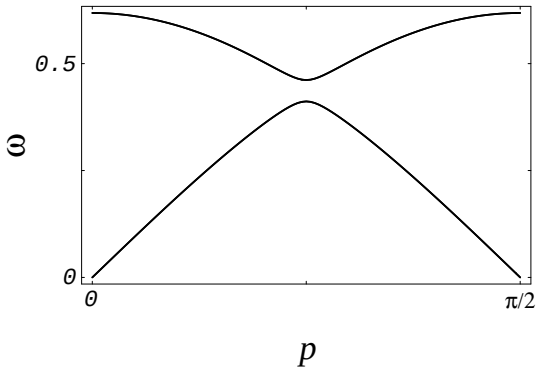

FIG. 4. The same figure as Fig.2, but with $\gamma_1 = \gamma_2 = -0.9$.

gapless spectrum of the system via the lowest-order spin-wave analysis. This is due to the fact that higher order quantum corrections play a crucial role whether or not the system is indeed gapless. What we would like to emphasize in this section is that the lowest mode has a linear spectrum, for which we are ensured to use non-linear sigma model techniques in order to investigate the characteristic properties of the models.

IV. NON-LINEAR SIGMA MODEL APPROACH

As was shown in the previous section, the spin excitations in both models A and B are characterized by the linear spectrum in the low energy regime. This suggests that we can map these models to O(3) non-linear sigma model (NLSM) in order to incorporate the quantum effects in a leading order approximation. Although the NLSM has been successfully applied to the usual uniform spin chain [2–5], there appear in the present models some other massive modes in addition to the lowest massless spin excitations, making the problem somewhat complicated. Therefore, it is not straightforward how to incorporate the effects of massive modes into the massless mode to obtain the effective NLSM. In this section, we propose a way to treat such effects, following the method recently developed in ref. [21] for spin-ladder systems.

The starting action is

$$S = S_B + S_H, \tag{4.1}$$

where

$$S_B = -i\sum_{j=1}^{N_a}(-)^{j+1}s_j w[\boldsymbol{n}(j)],$$
$$S_H = \frac{1}{2}\sum_{j=1}^{N_a} J_j s_j s_{j+1}\int d\tau\left[\boldsymbol{n}(j+1)-\boldsymbol{n}(j)\right]^2. \tag{4.2}$$

In the following, we would like to treat the two models separately.

A. Model A

For the Model A, the spin-wave spectrum has a three-band structure when $s_1 \neq s_2$. Therefore, we introduce the sigma-model fields as,

$$\boldsymbol{n}(3j+a) = \boldsymbol{m}(3j+a) + (-)^{3j+a+1}a_0\boldsymbol{l}_a(3j+a), \tag{4.3}$$

where a_0 is a lattice constant, $j = 0, 1, \cdots, N-1$ and $a = 1, 2, 3$. Note that whether the present models are massive or massless is essentially determined by the coefficient of the topological term, and may not be sensitive to how many fields we consider in the effective theory. However, it is expected that the introduction of three kind of fields l_1, l_2 and l_3 improves our low-energy effective theory, by incorporating the effects due to the massive modes to some extent: e.g. a better approximation may be obtained for the spin-wave velocity, as is seen below. In what follows we assume that the several fields thus introduced are sufficiently smooth functions so that we can take the continuum limit of them.

First, let us derive the expression for the Berry phase term in the continuum limit,

$$\begin{aligned} S_B = & \sum_{a=1}^{3}\sum_{j=0}^{N-1}(-)^{a+1}is_a \\ & \times\{\omega[\boldsymbol{n}(6j+a+3)]-\omega[\boldsymbol{n}(6j+a)]\} \\ = & \sum_{a=1}^{3}\sum_{j=0}^{N-1}(-)^{a}is_a \\ & \times\int d\tau\delta\boldsymbol{n}(6j+a)\cdot[\boldsymbol{n}(6j+a)\times\partial_\tau\boldsymbol{n}(6j+a)], \end{aligned} \tag{4.4}$$

where $s_a = s_1, s_2, s_2$ for $a = 1, 2, 3$, respectively, and $\delta\boldsymbol{n}(6j+a) \equiv \boldsymbol{n}(6j+a+3) - \boldsymbol{n}(6j+a)$. We replace the difference by the differentiation, $\delta\boldsymbol{n}(6j+a) \sim 3a_0\partial_x\boldsymbol{m}(6j+a) + (-)^a 2a_0\boldsymbol{l}_a(6j+a) + O(a_0^2)$, where a_0 is

the lattice constant. Substituting this formula, we then have

$$S_B = \frac{is}{2}\int d^2x \boldsymbol{m}\cdot(\partial_x\boldsymbol{m}\times\partial_\tau\boldsymbol{m}) + is_2\sum_a\int d^2x f_a\boldsymbol{l}_a\cdot(\boldsymbol{m}\times\partial_\tau\boldsymbol{m}), \quad (4.5)$$

where $s = s_1$ and

$$\boldsymbol{f} = \frac{1}{3}\begin{pmatrix}\alpha\\1\\1\end{pmatrix}, \quad (4.6)$$

with α defined in eq.(3.6).

Let us next take the continuum limit of interaction terms,

$$S_H = \frac{J}{2}\sum_{a=1}^{3}\sum_{j=0}^{2N-1} s_a s_{a+1} \times\int d\tau\left[\boldsymbol{n}(3j+a+1)-\boldsymbol{n}(3j+a)\right]^2. \quad (4.7)$$

Here, note that $\boldsymbol{n}(3j+a+1)-\boldsymbol{n}(3j+a)\sim a_0\partial_x\boldsymbol{m}(3j+a)+a_0(-)^{3j+a}\left[\boldsymbol{l}_{a+1}(3j+a)+\boldsymbol{l}_a(3j+a)\right]+O(a_0^2)$. Substituting this expression and neglecting oscillating terms, we have

$$S_H = \frac{Ja_0s_2^2}{2}\int d^2x\big[K(\partial_x\boldsymbol{m})^2 + \sum_a g_a\boldsymbol{l}_a\cdot\partial_x\boldsymbol{m}+\sum_{a,b}\boldsymbol{l}_aL_{ab}\boldsymbol{l}_b\big], \quad (4.8)$$

where $K=(2\alpha+1)/3$, $\boldsymbol{g}^t=(0,0,0)$ and

$$L = \frac{1}{3}\begin{pmatrix}2\alpha & \alpha & \alpha\\ \alpha & 1+\alpha & 1\\ \alpha & 1 & 1+\alpha\end{pmatrix}. \quad (4.9)$$

Here we have introduced $\boldsymbol{g}$ for later convenience (Model B).

Integrating the field $\boldsymbol{l}$, we end up with the effective Lagrangian density for $\boldsymbol{m}$,

$$\mathcal{L} = \frac{1}{2g}\left[v(\partial_1\boldsymbol{m})^2+\frac{1}{v}(\partial_2\boldsymbol{m})^2\right] + \frac{\theta}{8\pi}\epsilon_{\mu\nu}\boldsymbol{m}\cdot(\partial_\mu\boldsymbol{m}\times\partial_\nu\boldsymbol{m}), \quad (4.10)$$

where

$$\theta = 2\pi is\left(1+\frac{s_2}{s}\boldsymbol{g}^tL^{-1}\boldsymbol{f}\right),$$
$$g = \frac{1}{s_2}\frac{1}{\sqrt{\left(K-\frac{1}{4}\boldsymbol{g}^tL^{-1}\boldsymbol{g}\right)\boldsymbol{f}^tL^{-1}\boldsymbol{f}}},$$
$$v = Ja_0s_2\sqrt{\frac{K-\frac{1}{4}\boldsymbol{g}^tL^{-1}\boldsymbol{g}}{\boldsymbol{f}^tL^{-1}\boldsymbol{f}}}, \quad (4.11)$$

provided that L is a symmetric matrix. For the Model A, by the use of the following inverse matrix of L defined in eq.(4.9)

$$L^{-1} = \frac{3}{4\alpha}\begin{pmatrix}\alpha+2 & -\alpha & -\alpha\\ -\alpha & \alpha+2 & \alpha-2\\ -\alpha & \alpha-2 & \alpha+2\end{pmatrix}, \quad (4.12)$$

we have the following formula,

$$\theta = 2\pi is_1,$$
$$g = \frac{2}{s_2}\frac{3}{\sqrt{(2\alpha+1)(\alpha^2-2\alpha+4)}},$$
$$v = 2Ja_0s_2\sqrt{\frac{2\alpha+1}{\alpha^2-2\alpha+4}}. \quad (4.13)$$

It should be noted that in the case of $s_1=s_2\equiv s$, the above formulae reduce to those of the uniform spin-s spin chain, $\theta=2\pi is$, $g=2/s$ and $v=2Ja_0s$.

It is interesting to compare the formula (4.13) as those in Appendix A, which was previously obtained by assuming a single l-field (i.e., neglecting the effect of massive modes) [15]. The coefficient of the topological term is the same, $\theta=\widetilde{\theta}$, which makes the above formula reliable. The difference of the bulk quantities appears in the factors depending on α. From Table I, we found v closer to the value $v_{\rm sw}$. We can thus see that the approximation is improved by the introduction of three l-fields rather than a single l-field.

s_1		1/2	1	3/2	2	5/2
	$v_{\rm sw}$	1.000	1.061	0.878	0.707	0.582
$s_2=1/2$	v	1	1.113	1	0.866	0.761
	$\widetilde{v}$	1	1.25	1.4	1.5	1.571
	$v_{\rm sw}$	1.488	2.000	2.179	2.121	1.952
$s_2=1$	v	1.569	2	2.219	2.236	2.138
	$\widetilde{v}$	1.6	2	2.286	2.5	2.667

TABLE I. Spin-wave velocity for the Model A. The velocity denoted by $v_{\rm sw}$ is calculated by the spin-wave dispersion relation $\omega\sim v_{\rm sw}p$ for small p. It is compared with v given by eq.(4.13) in sec. IV. For reference, we also show $\widetilde{v}$ given by eq.(A1) for which the effects of massive modes are neglected.

Based on the above observations, we now arrive at the following conclusion for the Model A. The topological term is controlled only by the spin s_1, and this characteristic property is independent of the approximations we have used. Namely, if $s_1=$ integer (half-integer), the model is to be massive (massless). This is indeed consistent with the result by Lieb-Shultz-Mattis theorem in sec.II.

B. Model B

In the spin-wave analysis, we have found a two-band structure in the spectrum for the Model B, and so we here introduce the fields,

$$\boldsymbol{n}(j) = \boldsymbol{m}(j) + (-)^{j+1} a_0 \times \begin{cases} \boldsymbol{l}_1(j) & \text{for } j = 1,2 \\ \boldsymbol{l}_2(j) & \text{for } j = 3,4 \end{cases} \pmod 4 . \tag{4.14}$$

Manipulations for passing to the continuum limit are performed in parallel to the Model A. First, note that the continuum limit of the Berry phase terms takes the same form as eq.(4.5), but with

$$s = \frac{s_1 + s_2}{2}, \quad \boldsymbol{f} = \frac{1}{2} \begin{pmatrix} \alpha \\ 1 \end{pmatrix}. \tag{4.15}$$

Here, subscript a in eq.(4.5) runs from 1 to 2, because we have two modes now. Next, interaction terms are also calculated in the same form as eq.(4.8) for which the corresponding parameters are given as

$$\begin{aligned} K &= \frac{1}{4}\left(\Gamma_1 \alpha^2 + 2\Gamma\alpha + \Gamma_2\right), \\ \boldsymbol{g} &= \begin{pmatrix} \Gamma\alpha - \Gamma_1\alpha^2 \\ \Gamma\alpha - \Gamma_2 \end{pmatrix}, \\ L &= \frac{1}{2} \begin{pmatrix} 2\Gamma_1\alpha^2 + \Gamma\alpha & \Gamma\alpha \\ \Gamma\alpha & 2\Gamma_2 + \Gamma\alpha \end{pmatrix}, \end{aligned} \tag{4.16}$$

where $\Gamma_i \equiv 1 - \gamma_i$ and $\Gamma \equiv 1 + (\gamma_1 + \gamma_2)/2$.

It is straightforward to derive the explicit formulae for general γ_1 and γ_2, by eq.(4.11). However, their appearance is rather complicated generally, so that we here write down them for the simple case $\gamma_1 = \gamma_2 \equiv \gamma$. We thus have

$$\begin{aligned} \theta &= \pi i (s_1 + s_2) \frac{4(1+\gamma) s_1 s_2}{(s_1+s_2)^2 + \gamma(s_1 - s_2)^2}, \\ g &= \frac{1}{s_1 s_2} \frac{(s_1+s_2)^2 + \gamma(s_1-s_2)^2}{\sqrt{(1+\gamma)[(s_1+s_2)^2 + \gamma(s_1^2 - 6s_1 s_2 + s_2^2)]}}, \\ v &= 4Ja_0 s_1 s_2 \sqrt{\frac{(1-\gamma)(1-\gamma^2)}{(s_1+s_2)^2 + \gamma(s_1^2 - 6s_1 s_2 + s_2^2)}}. \end{aligned} \tag{4.17}$$

Now we wish to discuss the above formulae in several limiting cases. First, by setting $s_1 = s_2 = s$, they are reduced to $\theta = 2\pi i s(1+\gamma)$, $g = 2/s \times (1-\gamma^2)^{-1/2}$ and $v = 2Ja_0 s(1-\gamma^2)^{1/2}$, i.e, the usual formula for the uniform chain with bond-alternation. Next set $\gamma = 0$ for arbitrary s_1 and s_2. Then we have

$$\begin{aligned} \theta &= 4\pi i \frac{s_1 s_2}{s_1 + s_2}, \\ g &= \frac{s_1 + s_2}{s_1 s_2}, \\ v &= 4Ja_0 \frac{s_1 s_2}{s_1 + s_2}, \quad \text{for } \gamma = 0, \end{aligned} \tag{4.18}$$

We predict from this expression that *at $\gamma = 0$ the system is massive in general*. For example, $\theta = 4\pi i/3$ in the case $s_1 = 1/2$ and $s_2 = 1$. Note that the bulk quantities g and v are different from $\widetilde{g}$ and $\widetilde{v}$, respectively, defined by eq.(A2) which were previously derived [15] by neglecting massive modes from the beginning. On the other hand the coefficient of the topological term is the same in both cases, $\theta = \widetilde{\theta}$. By observing that v reproduces $v_{\rm sw}$ exactly in Table II, we naturally expect that the assumption (4.14) in our approach works rather well, making the above formula more reliable than the previous treatment with a single-l field approximation.

s_1		1/2	1	3/2	2	5/2
	$v_{\rm sw}$	1.000	1.333	1.500	1.600	1.666
$s_2 = 1/2$	v	1	1.333	1.5	1.6	1.667
	$\widetilde{v}$	1	1.491	1.936	2.332	2.687
	$v_{\rm sw}$	1.333	2.000	2.400	2.666	2.857
$s_2 = 1$	v	1.333	2	2.4	2.667	2.857
	$\widetilde{v}$	1.491	2	2.500	2.981	3.440

TABLE II. Spin-wave velocity for the Model B. Parameters are same as Table I, but with v given by eq.(4.17), and $\widetilde{v}$ given by eq.(A2).

Next, let us discuss the effects of the bond-alternation. First, we recall that for the usual uniform spin-s chain (see the above formula for $s_1 = s_2$ case), $\theta = 0 \to 4\pi i s$ if γ varies $\gamma = -1 \to 1$. Namely, the model realizes $2s$ massless points during this process [22]. However, it is difficult in general to predict the exact value of the bond-alternation parameter γ which brings about massless phases. For example, when $s = 1$, it is predicted by Affleck and Haldane [22] that a massless phase occurs at $\gamma = 1/2$, while the numerical calculation suggests a different value $\gamma = 0.25$ [23]. This is because for systems with explicitly broken translational symmetry, there are no strong restrictions by this symmetry and the coefficient of the topological term can take arbitrary values. This makes such values less reliable. Nevertheless it is believed that the number of massless points predicted by sigma model techniques itself should be correct, which has been indeed realized for the $s = 1$ case by numerical calculations [23].

Keeping this in mind, we would like to observe how the topological term θ behaves for for $s_1 \neq s_2$ case. From eq.(4.17), we can see that θ is an increasing function of γ,

$$\theta = 0 \to \pi i (s_1 + s_2) \frac{4 s_1 s_2}{s_1^2 + s_2^2}, \tag{4.19}$$

according to $\gamma = -1 \to 1$. For example, in Fig.5, we explicitly show θ (see the curve (a) in the figure) as a

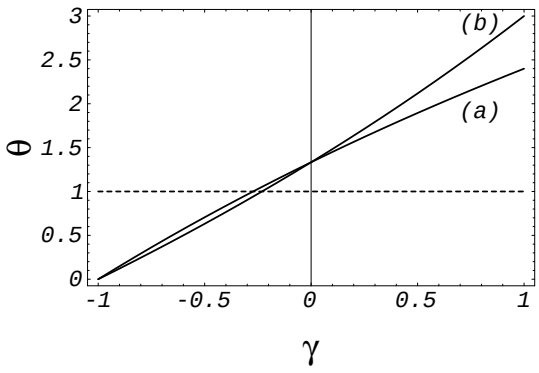

FIG. 5. (a) θ and (b) $\widetilde{\theta}$ in unit πi as functions of γ for $s_1 = 1/2$ and $s_2 = 1$.

function of γ in the case $s_1 = 1/2$ and $s_2 = 1$. We can see that at $\gamma \sim -0.273$, θ becomes 1 and massless phase is expected. It is interesting to compare this value with the numerical one $\gamma \sim -0.13$ in ref. [16]. This difference is not serious, as has been already discussed. What we are interested in is mainly how many times we expect massless phases in varying the bond-alternation parameter. Indeed, the conclusion of Tonegawa et al [16] is that there occurs only one massless phase in the whole antiferromagnetic region of γ, which is consistent with our results.

As we have now two kind of spins, it is interesting to study an extreme case where the difference between the two spins is large. Set, e.g, $s_2 \to \infty$, and we have $\theta \to 4\pi i s_1$ (and $g \to 0$) near $\gamma = 1$. In this limit, therefore, we have $2s_1$ massless points during the process $\gamma = -1 \to 1$. Namely, it turns out that smaller spin solely controls the number of the massless points.

Finally, we would like to compare the present result with the previous one (A2) which was derived by neglecting the effects of the massive spin modes. It turns out from (A2) that $\widetilde{\theta} = 0 \to 2\pi i(s_1 + s_2)$ for $\gamma = -1 \to 1$. Therefore, in the case that s_1 and s_2 are the same type of spins (integers or half-integers) the model has $s_1 + s_2$ massless points, while it may have $s_1 + s_2 - 1$ massless points in the case where the spins are of different type (the $\gamma = 1$ point cannot be classified as a massless point because the system is separated into disconnected dimers there). In Fig.5, we present $\widetilde{\theta}$ for reference, from which we see that behavior near $\gamma = 1$ is different from that of θ. However, the value of γ which gives $\widetilde{\theta} = 1$ is similar to that for θ in this case. In general, $\theta \leq \widetilde{\theta}$ at $\gamma = 1$, where equality holds only if $s_1 = s_2$. This discrepancy becomes more serious if the difference between the two spins s_1 and s_2 becomes larger.

Then the question is which formula is more reliable. In table III, we compare the spin-wave velocities calculated by means of the above two methods in case of the finite bond-alternation, corresponding to Figs.3 and 4. It is clearly seen from this table as well as Table II that not

s_1		1/2	1	3/2	2	5/2
	$v_{\rm sw}$	0.436	0.335	0.279	0.255	0.242
$\gamma = 0.9$	v	0.436	0.336	0.279	0.255	0.242
	$\widetilde{v}$	0.436	0.722	1.089	1.504	1.952
	$v_{\rm sw}$	0.436	0.614	0.748	0.859	0.955
$\gamma = -0.9$	v	0.436	0.614	0.748	0.859	0.955
	$\widetilde{v}$	0.436	0.591	0.689	0.768	0.837

TABLE III. Spin-wave velocity for the Model B with bond-alternation. The spin s_2 is fixed as $s_2 = 1/2$, and other parameters are same as Table II.

only for $\gamma = 0$ but also for rather large γ, v in (4.17) exactly reproduces the spin-wave velocity $v_{\rm sw}$ calculated in the spin-wave analysis in the previous section. On the contrary, the velocity $\tilde{v}$ considerably deviates from $v_{\rm sw}$. Notice especially the difference between Figs.3 and 4. These figures tell us that the hybridization between two spin modes in Fig.3 is much larger than that in Fig.4. Therefore, if we naively neglect the massive mode, it may cause more serious errors for the former case. One can indeed see this fact in the above table: Namely, $\widetilde{v}$'s for $\gamma = 0.9$ is worse in general than those for $\gamma = -0.9$. Based on these observations, we believe that the present formulae eq.(4.17), which incorporate the effect of massive modes, provide more reliable results.

To conclude, we may predict how many massless phases we encounter when we vary γ from -1 to 1: Namely it is given by the number of odd-integers included in the region between 0 and $4s_1s_2(s_1 + s_2)/(s_1^2 + s_2^2)$. It may be an interesting issue to investigate this conjecture directly by numerical calculations. The simplest case is,

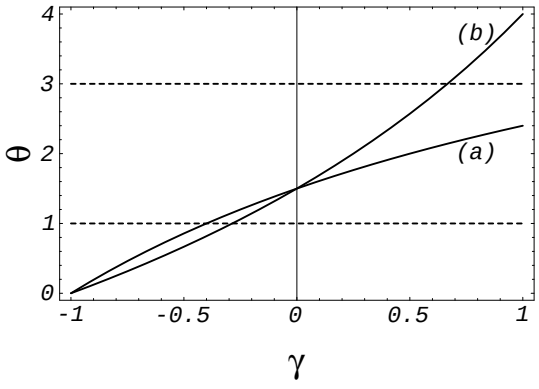

FIG. 6. (a) θ and (b) $\widetilde{\theta}$ in unit πi as functions of γ for $s_1 = 1/2$ and $s_2 = 3/2$.

for example, $s_1 = 1/2$ and $s_2 = 3/2$. The present formula (θ) predicts only one massless phase, while the previous formula ($\widetilde{\theta}$) predicts 2 massless phases, as can be seen from Fig.6.

V. SUMMARY

We have investigated two kind of alternating spin chains, both of which have singlet ground state. They are composed of a periodic array of two kind of spins. To analyze low-energy properties of these models, we have first studied spin-wave spectrum in detail. Introducing quantum fluctuations semiclassically, we have converted the low-energy spin mode to the O(3) non-linear sigma model. Analyzing the topological term in the sigma model, we have then clarified how the massless or massive excitations are developed reflecting the topological nature of the alternating spin system. Up to now, the alternating spin chains found experimentally have ferrimagnetic ground state. We think that the systems similar to those proposed here with singlet ground state could be fabricated experimentally, they would provide a new paradigm of the quantum spin systems, for which one may systematically observe the competition of the massive and massless phases.

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APPENDIX A: FORMULAE WITHOUT INTRODUCING MASSIVE MODES

In this appendix, in comparison with the formulae given in the text, we write down the expression without taking into account the effects of massive modes. We here quote the results obtained in the previous paper [15], in which a preliminary treatment was given for low-energy properties of the model. There, in order to map the model to the non-linear sigma model, only a single l-field was introduced, which means that the effects due to massive modes are neglected. One can find the detail of the derivation is given in the paper [15]. The formulae obtained are

$$\begin{aligned} \widetilde{\theta} &= 2\pi i s_1, \\ \widetilde{g} &= \frac{2}{s_2}\frac{3}{\alpha+2}, \\ \widetilde{v} &= 2Ja_0 s_2 \frac{2\alpha+1}{\alpha+1}, \end{aligned} \tag{A1}$$

for Model A, and

$$\begin{aligned} \widetilde{\theta} &= 2\pi i s_{\rm eff}(1+\gamma_{\rm eff}), \\ \widetilde{g} &= \frac{2}{s_{\rm eff}\sqrt{1-\gamma_{\rm eff}^2}}, \\ \widetilde{v} &= 2Ja_0 s_{\rm eff}\sqrt{1-\gamma_{\rm eff}^2}, \end{aligned} \tag{A2}$$

for Model B with $\gamma_1 = \gamma_2 \equiv \gamma$, where

$$\begin{aligned} s_{\rm eff} &= \frac{s_1+s_2}{2}, \\ \gamma_{\rm eff} &= \frac{(s_1+s_2)^2\gamma - (s_1-s_2)^2}{(s_1+s_2)^2 - (s_1-s_2)^2\gamma}. \end{aligned} \tag{A3}$$

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